The calculus of the electric potential and field intensity in multiple electrodes lateral tunneling transistors with double gate

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Abstract. The paper presents an adaptive over-relaxation method for calculating the electric potential and field intensity, for a complex tunnel transistor structure involving a split gate and a shielding boundary. The accuracy and speed of the method has been numerically tested and found satisfactory for the study of such devices by calculating the tunneling currents for the obtained potential distribution.

1. Introduction

This highly promising tunnel transistor structures have been intensely investigated in the last decade, for the future industrial application. Among the large variety of proposed models there are some with simple barrier [1], and others that include one or more quantum wells [2]. The first type is based on the modulation of the Fowler-Nordheim tunneling current by the electric field intensity created by an auxiliary electrode. The second type is based on the resonance effects between the quantum wells, as a significant tunneling current appears only if some quantum states equivalence is satisfied. An auxiliary electrode controls the resonance conditions, starting or stopping the tunneling current, so that the structure is easy to be used as a commutation device. Concerning the geometry, there are also several types of tunnel transistors. Thus, the most promising seems to be the vertical transistor where the electrodes are superposed, which allows a very good control of the thickness of the barrier layer and hence a good reproducibility for large scale integration [1],[3],[4][7],[8]. Also, lateral structures have been proposed, based on a Columbian barrier generated by a lateral p-n junction, which is easier to control by the gate electrode [5],[6]. There are also some mixed structures [2] where both vertical and horizontal geometries are used, and also some special devices as the magnetic tunnel transistor and the single electron transistor (SET) used as structures in scientific research [9].

The calculus of the tunneling currents in the tunnel transistors structures implies the previous calculation of the electric potentials or electric field intensity in all the points of the active domain, for various potentials applied on the electrodes.

These values will be used as an ansatz for the quantum mechanics calculations of the tunneling currents using either Schrödinger or Nordheim-Fowler type equations, and hence the static characteristics of the tunnel transistor for a given geometry and for certain materials of the structure.

The potentials in a lateral tunnel transistor type structure obeys the bi-dimensional Laplace equation:

$$\frac{\partial^2 V(x,y)}{\partial^2 x^2} + \frac{\partial^2 V(x,y)}{\partial^2 y^2} = 0 \tag{1.1}$$

with the boundary conditions (Dirichlet type) :

$$V(x,y)|_{\partial_i D} = a_i \quad , i = 1, 2, ..., n \tag{1.2}$$

where $\partial_i D$ is one of the n boundaries of the metallic electrodes or of the whole domain.

For simple systems with a certain symmetry it may be possible to analytically solve such an equation, but any change in the geometry would impose a new analytical calculation. For practical purpose, the mathematical modeling has to be numerically solved so that the some computer software should be used for a big number of models. In most of the cases, a rectangular bi-dimensional domain may be considered and a grid of equidistant points (nodes) chosen. If the axes origin is a corner of the rectangular domain and if there are N points in each direction, with the steps:

$h_x = \frac{x_{\max}}{N}$
$h_y = \frac{y_{\max}}{N}$

we may find the values of the potentials in the nodes: $V(x_i, y_i)$; $i = 1, 2, ..., N$; $j = 1, 2, ..., N$

The finite difference approximation of the eq. (1.1) leads to:

$$\begin{aligned} V(x_i, y_i) = & \frac{h_y^2}{2(h_x^2+h_y^2)}[V(x_{i-1}, y_j) + V(x_{i+1}, y_j)] \\ & + \frac{h_x^2}{2(h_y^2+h_x^2)}[V(x_i, y_{i-1})] + V(x_i, y_{i+1})] \end{aligned} \tag{1.3}$$

If $x_{\max} = y_{\max}$ (square domain) we have $h_x = h_y$ and the potential in a node is the mean of the potentials of its neighbors.

$$\begin{aligned} & V(x_i, y_i) = \tfrac{1}{4}[V(x_{i-1}, y_j) + V(x_i, y_{j-1}) \\ & + V(x_{i+1}, y_j) + V(x_i, y_{j+1})] \quad i, j = 1, 2, ..., N \end{aligned} \tag{1.4}$$

The errors are of the order $\mathcal{O}(h^2)$ so that an 100×100 points grid is adequate for most practical purposes. However, the equations system for such a grid has 10^4 equations and unknowns, which implies increased errors due their propagation and the often bad conditioning. That is why in many cases the direct solving of such a system is not the best choice, and the iterative methods are preferred.

Thus, a Jacobi iteration [10] will compute at the step $k+1$ the potential value from the neighborhood potentials calculated at step k :

$$\begin{aligned} & V^{(k+1)}(x_i, y_i) = \tfrac{1}{4}[V^{(k)}(x_{i-1}, y_j) + V^{(k)}(x_{i+1}, y_j) \\ & + V^{(k)}(x_i, y_{j-1}) + V^{(k)}(x_i, y_{j+1})] \end{aligned} \tag{1.5}$$

A better convergence is achieved if we include in the $k+1$ step the previously calculated values of the same step, according to the Gauss-Siedel algorithm [10]:

$$\begin{aligned} & V^{(k+1)}(x_i, y_i) = \tfrac{1}{4}[V^{(k+1)}(x_{i-1}, y_j) + V^{(k+1)}(x_i, y_{j-1}) \\ & + V^{(k)}(x_{i+1}, y_j) + V^{(k)}(x_i, y_{j+1})] \end{aligned} \tag{1.6}$$

The convergence may be further increased using an over-relaxation method, with a relaxation factor $\beta \in (1, 2)$ that may be experimentally determined:

$$\begin{aligned} & V^{(k+1)}(x_i, y_i) = (1-\beta)V^{(k)}(x_i, y_j) + \beta\tfrac{1}{4}[V^{(k+1)}(x_{i-1}, y_j) \\ & + V^{(k+1)}(x_i, y_{j-1})] + V^{(k)}(x_{i+1}, y_j) + V^{(k)}(x_i, y_{j+1}) \end{aligned} \tag{1.7}$$

This procedure may be much faster than Gauss-Siedel (which is equivalent with the $\beta = 1$ case) if a proper value of β is chosen so that, taking into account the speed of modern computers, it is suitable for tunneling transistors structures.

2. The electric potential distribution in the lateral tunneling transistor with four metallic electrodes

We propose a tunneling transistor structure with coplanar source, drain and gate as in figure 1. For a better control efficiency of the gate, it is split and symmetrically related to the source-drain region. The two halves are interconnected in a different plane at considerable distance from the main plane, to avoid tunneling, as in figure 2.

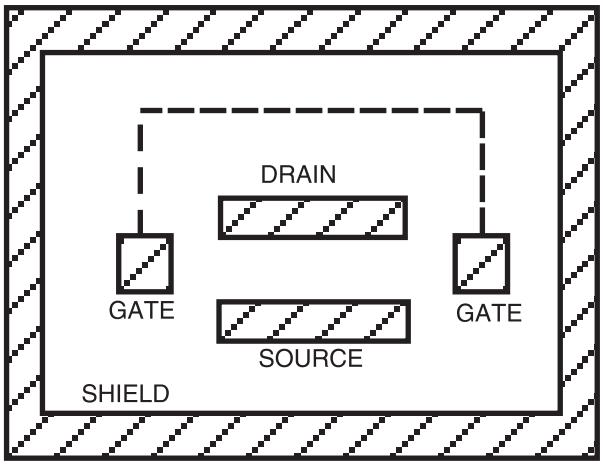

Figure 1. Top view of the proposed lateral transistor structure

Also, a grounding metallic shield avoids the influence between adjacent transistors and establish the boundary conditions for the second order elliptic partial derivative equation.

This geometry imposes the Dirichlet conditions for the partial derivative equation. We denote the following boundaries:

∂S -the source electrode domain and its boundary;

∂D -the drain electrode domain and its boundary;

∂G -the gain electrode domain and its boundary;

∂Sh - the shield electrode domain and its boundary;

Taking into account this geometry, we impose:

$$V(x_i, y_j) = V_S \quad , \quad \{x_i, y_j\} \in \partial S \tag{2.1}$$

$$V(x_i, y_j) = V_D \quad , \quad \{x_i, y_j\} \in \partial D \tag{2.2}$$

$$V(x_i, y_j) = V_G \quad , \quad \{x_i, y_j\} \in \partial G \tag{2.3}$$

$$V(x_i, y_j) = 0 \quad , \quad \{x_i, y_j\} \in \partial Sh \tag{2.4}$$

If we choose the axes origin in the left lower corner of the domain, the condition 2.4 becomes:

$V(x_i, 0) = 0 \quad , \quad i = 1, 2, ..., N$

$V(0, y_j) = 0 \quad , \quad j = 1, 2, ..., N$

$V(x_i, N) = 0 \quad , \quad i = 1, 2, ..., N$

$V(N, y_j) = 0 \quad , \quad j = 1, 2, ..., N$

Considering that the errors are indicated by the values variances from an iteration to another, we have to include in the algorithm the quantity:

$$\varepsilon_k = V^{(k+1)}(x_m, y_m) - V^{(k)}(x_m, y_m) \tag{2.5}$$

The point $\{x_m, y_m\}$ will characterize the errors evolution for the whole domain, as a "mean" value for the potentials variations. In practice we closed the midpoint of the

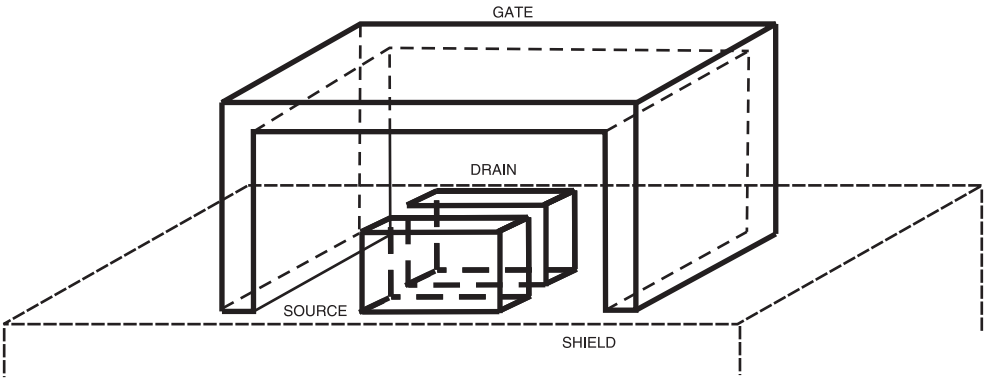

Figure 2. Lateral view of the proposed lateral transistor structure (the shield is partially shown)

domain and we supposed that the errors in all the other points are quite similar. A choice of a single point for this purpose is necessary for making a single evaluation at an iteration as a criterium for stopping the iterative process.

A more precise choice for the point where the error is evaluated should be one with a maximum absolute value, near one of the electrodes. Anyway, the errors may be kept much lower than the technological dispersion, as our experiments proved.

For accelerating the iterative process, we elaborated an adaptive algorithm, varying the relaxation factor β in accordance with the variance of ε_k , taking a medium start value $\beta_0 = 1.5$.

$$\beta_k = \beta_0 + E_{\max}(\varepsilon_{k+1} - \varepsilon_k) \tag{2.6}$$

The typical values of the relaxation factor β achieved for various geometries and electrodes potential is between 1.7 and 1.9. For a grid with $N = 100$, the number of iterations for a 10^{-4} precision goal is between 200 and 500 and the calculation time around some minutes.

3. The electric field intensity in the lateral tunneling transistor with four metallic electrodes

If the tunneling current calculus is based on the Schrdinger equation (the ab-initio method), only the potential distribution in the structure is needed. However, if the more efficient Nordheim-Fowler equations are directly used, they need the values of the electric field intensity. It may be calculated from the partial derivatives of the potential:

$$E_x(x_i, y_j) = -\frac{\partial V(x,y)}{\partial x}|_{x_i,y_j} \tag{3.1}$$

$$E_y = -\frac{\partial V(x,y)}{\partial y}|_{x_i,y_j} \tag{3.2}$$

Numerically, the mid-point formula of the derivative may be used, as it provides a good enough precision:

$$E_x(x_i, y_j) = -\frac{V(x_{i+1}, y_j) - V(x_{i-1}, y_j)}{2h} \tag{3.3}$$

$$E_y(x_i, y_j) = -\frac{V(x_i, y_{j+1}) - V(x_i, y_{j-1})}{2h} \tag{3.4}$$

For a better precision we experimented two supplementary methods that we shall describe . The first possibility is to use a classical polynomial interpolation (Lagrange-Neville for example):

$$P_j(x) = \sum_{i=1}^{N} V(x_i, y_j) \prod_{\substack{k=1 \\ k\neq i}}^{N} \frac{x - x_k}{x_i - x_k} \quad j = 1, 2, ..., N \tag{3.5}$$

$$P_i(y) = \sum_{j=1}^{N} V(x_i, y_j) \prod_{\substack{k=1 \\ k\neq j}}^{N} \frac{y - y_k}{y_j - y_k}; \quad i = 1, 2, ..., N \tag{3.6}$$

Expanding these expressions in the form:

$$P_j(x) = \sum_{i=1}^{N} a_{ij} x^i \quad ; \quad j = 1, 2, ..., N \tag{3.7}$$

$$P_i(y) = \sum_{j=1}^{N} b_{ij} y^j \quad ; \quad i = 1, 2, ..., N \tag{3.8}$$

the derivatives may be precisely calculated :

$$P_j^{'}(x) = \sum_{i=1}^{N} i a_{ij} x^{i-1} \quad ; \quad j = 1, 2, ..., N \tag{3.9}$$

$$P_i^{'}(x) = \sum_{j=1}^{N} j b_{ij} y^{j-1} \quad ; \quad i = 1, 2, ..., N \tag{3.10}$$

We obtain the electric field intensity components as

$$E_x(x_i, y_j) = \sum_{i=1}^{N} i a_{ij} x_i^{i-1} \quad ij = 1, 2, ..., N \tag{3.11}$$

$$E_y(x_i, y_j) = \sum_{j=1}^{N} j b_{ij} x_j^{j-1} \quad ij = 1, 2, ..., N \tag{3.12}$$

Although the procedure seems very precise due to the analytical derivation, our tests revealed that it may be used only for low values of N . The problem is generated by the equidistant points grid, which reveals the Runge phenomenon for high N values.

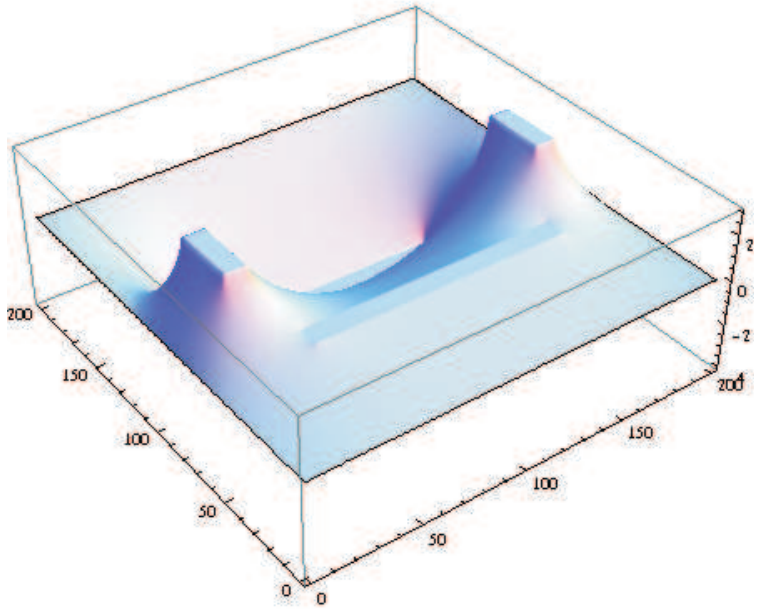

Figure 3. Three-dimensional representation of the potentials - source view

A second solution that was tested was the choose of the interpolation points according to the Chebyshev (or even Gauss-Lobatto) conditions.

$$x_k = \text{Int}\{N[1 - \cos(2k-1)\frac{\pi}{2N}]\} \tag{3.13}$$

$$y_l = \text{Int}\{N[1 - \cos(2l-1)\frac{\pi}{2N}]\} \tag{3.14}$$

This eliminates the Runge phenomenon but the complications of the algorithm were not sustained by a significant increase of the precision compared to the mid-point derivative.

4. Conclusions

We exemplify the described procedures using a 200x200 grid and the following potentials:
$V_D = -3V$
$V_S = 1V$
$V_G = 3V$

We choose a relaxation factor $\beta = 1.9$ and the error reference point at 100,100 imposing a 0.01 % precision goal. The potential calculated in this point after 330 iterations was -1.42714V and the previous iteration value was -1.42713V. The calculation time on a 3GHz computer in a Mathematica 7.0 environment was about 310 seconds. Of course, using a C++ environment, the speed would be up to ten times higher.

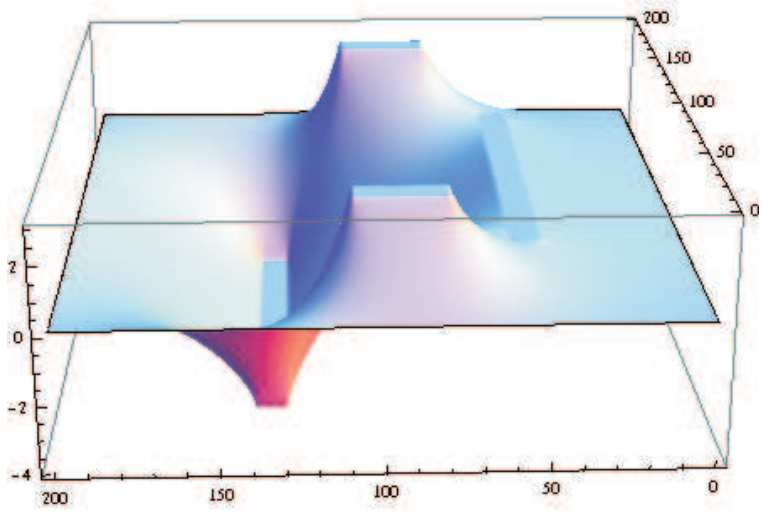

Figure 4. Three-dimensional representation of the potentials - lateral view

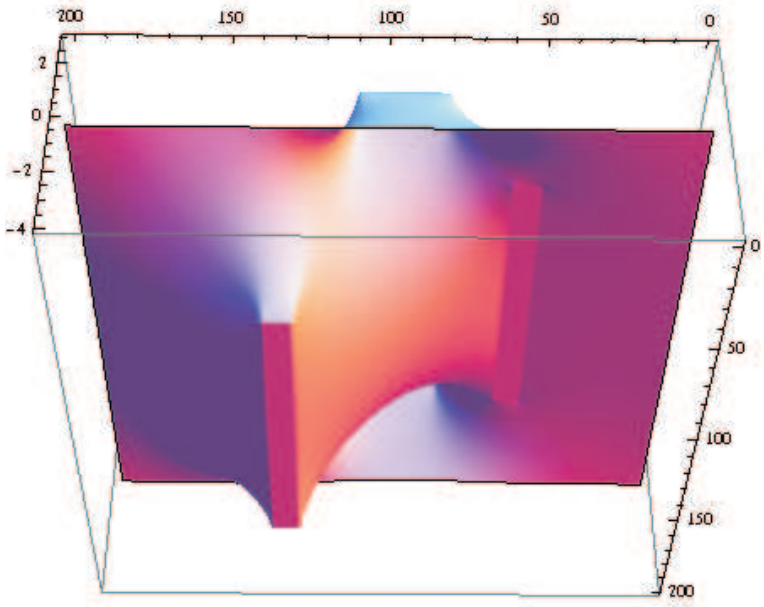

Figure 5. Three-dimensional representation of the potentials - bottom view

A sample of the potential values in a section with x=40 is the following
V(40,i)=0,0.0244191,0.0487992,0.0731018,0.0972886,0.121322,0.145164,0.168781,0.192136,
0.215195,0.237928,0.260304,0.282294,0.303873,0.325016,0.345701,0.365911,0.385628,
0.40484,0.423538,0.441713,0.459362,0.476485,0.493083,0.509163,0.524733,0.539802,
0.554382,0.568487,0.582129,0.59532,0.60807,0.620383,0.63226,0.643693,0.654667,
0.665159,0.675138,0.684575,0.693438,0.701706,0.709369,0.71643,0.722907,0.728828,
0.734227,0.739145,0.743621,0.747696,0.751408,0.754792,0.75788,0.760703,0.763286,
0.765653,0.767824,0.76982,0.771655,0.773345,0.774903,0.776341,0.77767,0.778898,
0.780034,0.781086,0.782061,0.782964,0.783802,0.78458,0.785301,0.785971,0.786593,
0.78717,0.787706,0.788204,0.788665,0.789094,0.789491,0.789859,0.7902,0.790516,
0.790807,0.791075,0.791323,0.79155,0.791758,0.791948,0.792121,0.792278,0.792419,
0.792545,0.792657,0.792755,0.792839,0.79291,0.792969,0.793015,0.793049,0.793071,
0.793081,0.793078,0.793064,0.793038,0.793,0.792949,0.792886,0.79281,0.792721,
0.792618,0.792501,0.79237,0.792223,0.79206,0.791881,0.791684,0.791469,0.791234,
0.790979,0.790702,0.790402,0.790077,0.789726,0.789347,0.788938,0.788497,0.788021,
0.787509,0.786956,0.786362,0.785721,0.785031,0.784287,0.783485,0.78262,0.781687,
0.78068,0.779593,0.778417,0.777146,0.77577,0.774279,0.772662,0.770906,0.768997,
0.76692,0.764657,0.762187,0.759488,0.756536,0.753302,0.749756,0.745863,0.741588,
0.736893,0.731738,0.726088,0.719907,0.713171,0.705863,0.697979,0.689529,0.680533,
0.671021,0.66102,0.650558,0.639656,0.628326,0.616573,0.604396,0.591788,0.578737,
0.56523,0.551252,0.53679,0.52183,0.50636,0.490372,0.473858,0.456815,0.439243,
0.421143,0.402521,0.383385,0.363748,0.343623,0.323027,0.301981,0.280507,0.258628,
0.236372,0.213767,0.190842,0.167631,0.144164,0.120478,0.0966066,0.0725862,0.0484534
,0.0242455,0

In figures 3-6 we also show a three-dimensional representation of the calculated potentials with different view points

We conclude that the over-relaxation method is well suited for the calculus of the potential distribution in a multiple electrodes structure with reasonable speed and accuracy, especially if the described adaptive algorithm for adjusting the relaxation factor is used.

Acknowledgments

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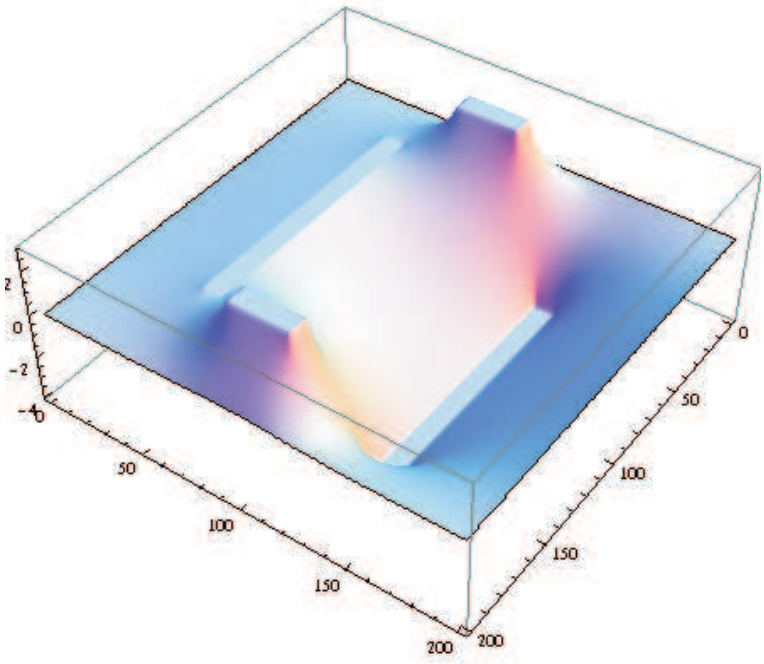

Figure 6. Three-dimensional representation of the potentials - drain view

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